Entropy and entanglement in polymer quantization

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Polymer quantization is as a useful toy model for the mathematical aspects of loop quantum gravity and is interesting in its own right. Analyzing entropies in the standard Hilbert space and the polymer Hilbert space we show that they converge in the limit of vanishing polymer scale. We derive a general bound that relates entropies of physically equivalent states in unitarily inequivalent representations.

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Statistical thermodynamics, quantum mechanics and information theory promoted entropy from an auxiliary variable of the mechanical theory of heat [1] to one of the most important quantities in science [2, 3]. Microscopic derivations of the thermodynamical entropy were, and still are, a major part of the statistical physics. Entropy and related quantities underpin most of the classical and quantum information theory [4]. Black hole thermodynamics [5] introduced the idea that an upper bound on the entropy of a system (and entanglement between the subsystems) scales with the area, and not with the volume. Formalized as a holographic principle, the area law was demonstrated in a variety of situations [6, 7], which include string and loop quantum gravity (LQG) [8] calculations of black hole entropy [5, 9] and related models [10].

LQG and the spin networks/ spin foams formalisms represent the idea of fundamental discreteness. They are conceptually and technically different from the usual quantum field theory on a space-time continuum. This difference leads to a number of questions. One of them [8, 11] is emergence of the semiclassical states of quantum gravity. These states have to enable the space-time continuum view and the ensuing construction of a field theory. Investigation of this problem and the associated mathematical issues were one of the motivation to study the polymer quantization of a single non-relativistic particle [11] as a useful toy model.

Another question pertains to the validity of holographic principle(s) and compatibility of the entropy calculations across different quantization schemes. Recent advances in coupling gravity and matter [12] in LQG [8] make it necessary to re-consider holography in these systems, which is derived separately in the gravity and the matter sectors. One can wonder if two unitarily inequivalent quantization schemes give compatible predictions for observables, are the predicted entropies "close"? While the desirable answer is "yes", its validity is neither obvious nor guaranteed. Again, the polymer quantization provides a convenient model setting to study this problem.

We demonstrate that, if the Schrödinger and the polymer schemes give "close" (to be precisely defined below) predictions for fundamental observables, their predictions of entropy are close. The two entropies coincide in the continuum limit of the polymer quantization. We illustrate this by comparing the entanglement entropy in the ground state of coupled harmonic oscillators in the two schemes.

The rest of this paper is organized as follows. After a brief review of the polymer quantization we describe our main result, outline the calculational techniques for Gaussian states, and present the example. We conclude with discussing possible limitations and future directions.

I. REVIEW OF POLYMER QUANTIZATION

A useful starting point is a unitary Weyl (displacement) operator,

$$\hat{W}(q,k)^\dagger = \hat{W}(-q,-k), \tag{1}$$

where q and k are the translation an boost parameters, respectively. The Weyl operator can be expressed as a product of the translation and boost operators,

$$\hat{W}(q,k) = e^{\frac{i}{2}qk}\hat{V}(q)\hat{U}(k) = \hat{W}(q,k) = e^{-\frac{i}{2}qk}\hat{U}(k)\hat{V}(q), \tag{2}$$

Here and in the following we set $\hbar = 1$.

In the standard Schrödinger representation these unitary operators are generated by the self-adjoint position and momentum operators,

$$\hat{V}(q) = e^{iq\hat{p}}, \qquad \hat{U}(k) = e^{ik\hat{x}}, \tag{3}$$

and the Weyl operator acts on wave functions as

$$\hat{W}(q,k)\psi(x) = e^{-\frac{i}{2}kq}e^{ikx}\psi(x+q). \tag{4}$$

The polymer representation is built around (Harald) Bohr compactification of the real line [14, 15]. A slightly different construction is possible by noting that the (position) space $\mathcal{H}_{\text{poly}}$ is spanned by the basis states $|x\rangle$,

$$\psi_x(x') = (x'|x\rangle = \langle x'|x\rangle = \delta_{x'x}, \tag{5}$$

where δ is Kronicker's delta, and the various bracket signs are explained below. Countable superpositions of these states,

$$|\Psi\rangle = \sum_{x\in\gamma}\psi(x)|x\rangle, \tag{6}$$

where γ is a countable set (a "graph" [11]) and functions ψ satisfy certain fall-off conditions, form a space of cylindrical functions Cyl_γ. The infinite-dimensional space Cyl

is a space of functions that are cylindrical with respect to some graph. The Hermitian inner product on Cyl follows from Eq. (5),

$$\langle\Psi|\Psi'\rangle = \sum_{x\in\gamma\cap\gamma'} \psi^*(x)\psi'(x). \tag{7}$$

The Cauchy completion of Cyl is $\mathcal{H}_{\rm poly}$, and the the triplet of spaces

$$\mathrm{Cyl} \subset \mathcal{H}_{\rm poly} \subset \mathrm{Cyl}^\star, \tag{8}$$

where $\mathrm{Cyl}^\star$ is an (algebraic) dual of Cyl, shares similarities with the construction of the physical space of LQG [11]. The questions of topology are discussed in [11, 17, 18]. Dual elements are denoted by $(\Upsilon|$, and their action on the elements of $\mathcal{H}_{\rm poly}$ by $(\Upsilon|\Psi\rangle \equiv \Upsilon(\Psi)$. The inner product defines a dual element by

$$\Phi(\Psi) \equiv \langle\Phi|\Psi\rangle. \tag{9}$$

We introduce the momentum dual states $(p| \in \mathrm{Cyl}^\star$ by

$$(p|x\rangle \equiv e^{-ipx}. \tag{10}$$

Hence

$$(p| = \sum_{x\in\mathbb{R}} e^{-ipx}\langle x|, \qquad \psi(p) = (p|\Psi\rangle. \tag{11}$$

In the "position representation" that was described so far the operator $\hat{U}(k)$ has a self-adjoint generator $\hat{x}$, that acts by multiplication and has normalized eigenstates,

$$\hat{x}|x\rangle = x|x\rangle. \tag{12}$$

However, since $|x_j\rangle$ and $\hat{V}(q)|x_j\rangle$ are orthogonal to each other no matter how small the translation is, the translation operator is not weakly continuous and the momentum operator is undefined. Similarly, while it is easy to show that the usual relation

$$(p|\hat{V}(q) = e^{ipq}(p| \tag{13}$$

holds, it does not correspond to any state of Cyl.

On the other hand, a momentum representation is spanned by the states $|k_j\rangle$. In this case there exists a self-adjoint momentum operator with normalizable eignestates, but the position operator is undefined. Since the polymer representation(s) are not weakly continuous, they do not satisfy the conditions of the Stone-von Neumann [13] theorem and thus are not unitarily equivalent to the Schrödinger representation [11, 14].

The two constructions of the $\mathcal{H}_{\rm poly}$ allows the most extreme expression [14] of Bohr's complementarity [16]. Failure of the weak continuity makes it into a convenient toy model of LQG, and it was recently studied both as such and in its own right [11, 17–19]. Moreover, the polymer quantization and its generalization to a scalar field were applied to the problems of quantum cosmology and spherically-symmetric collapse [20].

Fell's theorem [21] guaranties that, although two representations may be unitarily inequivalent, by using a finite number of finite-precision expectation values of observables it is impossible to distinguish between the two. More precisely, for a state ρ_1 of one of the representations, a finite set of operators A_i (belonging to the Weyl algebra) whose expectations are calculated on that state, and the set of tolerances ϵ_i there exists a "physically equivalent" state ρ_2 on another representation resulting in the expectation values that differ from the first set by less than the prescribed tolerances. Since its proof is not constructive, an explicit construction of states and operators is needed in each case.

While a mathematically rigorous construction involves a multi-scale lattice [17], we follow the approach of [11] and will work with a regular lattice γ, where the neighboring points have a fixed spacing μ. An effective momentum operator is introduced through the finite difference

$$\hat{p}_\mu \equiv -\frac{i}{2\mu}\big(\hat{V}(\mu) - \hat{V}^\dagger(\mu)\big). \tag{14}$$

The limit $\mu \to 0$ in the Schrödinger representation gives the usual momentum operator $\hat{p}$. Similarly, its square is

$$\hat{p}_\mu^2 \equiv (\hat{p}_\mu)^2 = \frac{1}{4\mu^2}\big(2 - \hat{V}(2\mu) - \hat{V}(-2\mu)\big) \tag{15}$$

The operators are self-adjoint [11, 17]. However, $\hat{p}_\mu^2$ is not positive on a general Cyl_γ even if it is a regular lattice. For example, for a state [17]

$$|\Psi\rangle = \sum_{x\in\gamma} e^{ikx} e^{x^2/2d^2}|x\rangle \tag{16}$$

the expectation value $\langle\Psi|\hat{p}_\mu^2|\Psi\rangle$ is real only for a symmetric graph, i.e. $x \in \gamma \Leftrightarrow -x \in \gamma$. We will restrict ourselves only to such graphs.

It follows from Eq (15) that $\hat{p}_\mu^2$ skips the neighboring lattice sights when acting on states, hence its eignefunctions can have support on either even- or odd-numbered sights $n\mu$, $n \in \mathbb{Z}$. As a result, using $\hat{p}_\mu^2$ as the kinetic terms for a Hamiltonian $\hat{H}_\mu$ leads to a double degeneracy of the eigenstates [11, 19] when compared with the Schrödinger representation. Without appealing to it, one can note that the state counting gives twice the semiclassical result $\int dp\,dx/2\pi$. Depending on one's goals it is possible either to adjust the state counting or to introduce a kinetic operator [11]

$$\hat{K}_\mu \equiv \widehat{p^2}_\mu \equiv \frac{1}{\mu^2}\big(2 - \hat{V}(\mu) - \hat{V}(-\mu)\big), \tag{17}$$

The commutation relations between the operators are

$$[\hat{x}, \hat{V}(\mu)] = -\mu\hat{V}(\mu), \tag{18}$$

$$[\hat{x}, \hat{p}_\mu] = \frac{i}{2}\big(\hat{V}(\mu) + \hat{V}(-\mu)\big) = i\big(1 - \tfrac{1}{2}\mu^2\hat{K}_\mu\big), \tag{19}$$

$$[\hat{p}_\mu, \hat{K}_\mu] = 0. \tag{20}$$

A key step in extracting physical predictions in the polymer quantization is to consider the shadow states [11], that realize the physically equivalent state on $\mathcal{H}_{\rm poly}$. These are projections of the elements of $\mathrm{Cyl}^\star$ onto Cyl_γ,

$$(\Phi| = \sum_{x\in\mathbb{R}} \Phi^*(x)(x| \to |\Phi^{\rm shad}\rangle = \sum_{x\in\gamma}\Phi(x)|x\rangle. \tag{21}$$

Using these states it is possible to explicitly demonstrate physical indistinguishability of the predictions of the polymer and Schrödinger quantizations, as mandated by Fell's theorem.

II. ENTROPY

Unlike observables that can be constructed from the Weyl algebra, there is no existence result that guaranties equivalence of the predictions for entropy. Moreover, it is known [3] that entropy is not a continuous function, and without additional restrictions there are states of infinite entropy in a neighborhood of any state.

Consider a Schrödinger state

$$\rho = \sum_i w_i |\psi_i\rangle\langle\psi_i|, \tag{22}$$

where the $|\psi_i\rangle$ form an orthogonal basis. If this basis is formed by the eigenstates of some operator, and its polymer counterpart has the corresponding eigenbasis $|\Psi_i\rangle$, then the decomposition

$$\rho^0_{\rm poly} = \sum_i w_i |\Psi_i\rangle\langle\Psi_i| \tag{23}$$

trivially has the same entropy, but it is not guaranteed that the expectation variables of all the observables of interest are close.

The shadow analog

$$\rho_{\rm poly} = \sum_i w_i |\Psi(\mu)_i\rangle\langle\Psi(\mu)_i|, \tag{24}$$

with $|\Psi(\mu)_i\rangle$ being the normalized shadow states $|\Psi(\mu)_i^{\rm shad}\rangle$, that are close "approximations" of the states $|\psi_i\rangle$ in the sense of Fell's theorem. The shadow states are not in general orthogonal [11], making the entropy estimation more complicated.

Concavity of entropy [3] leads to an inequality that in our case reads as

$$S(\rho_{\rm poly}) \le -\sum w_i \log w_i = S(\rho), \tag{25}$$

This result holds for any two representations were the equivalent state of any $|\psi\rangle$ is pure.

Consider a (completion of the) linear span of the shadow states $|\Psi(\mu)_i\rangle$ as a Hilbert space $\mathcal{K}_\mu$. It is a separable Hilbert space and has an orthonormal basis, which can be built from the states $|\Psi(\mu)_i\rangle$ by the Gramm-Schmidt procedure. As the lattice scale μ decreases, the shadow states tend to an orthonormal system,

$$\lim_{\mu\to 0}\langle\Psi(\mu)_j|\Psi(\mu)_k\rangle = \delta_{jk}. \tag{26}$$

hence if the basis vector $|i_\mu\rangle \in \mathcal{K}_\mu$ is obtained from $|\Psi(\mu)_i\rangle$, then

$$|\Psi(\mu)_k\rangle = \sum_l c^\mu_{kl}|l_\mu\rangle, \qquad \lim_{\mu\to 0} c^\mu_{kl} = \delta_{kl}. \tag{27}$$

All separable Hilbert spaces are isometrically isomorphic, so for every μ we can introduce a unitary operator $U_\mu : \mathcal{K}_\mu \to \mathcal{K}$, where $\mathcal{K}$ is some "standard" Hilbert space. Then

$$U_\mu|l_\mu\rangle = |l\rangle \in \mathcal{K}, \qquad U_\mu|\Psi(\mu)_k\rangle = \sum_l c^\mu_{kl}|l\rangle. \tag{28}$$

Consider two density operators on the space $\mathcal{K}$,

$$\bar\rho = \sum_i w_i|i\rangle\langle i|, \qquad \rho_\mu = \sum_{ikl} w_i c^{\mu *}_{ik} c^\mu_{il}|k\rangle\langle l|, \tag{29}$$

where $S(\bar\rho)=S(\rho)$ and $S(\rho_{\rm poly}) = S(\rho_\mu)$. Using Eq. (27) we find that

$$\lim_{\mu\to 0} \mathrm{tr}|\bar\rho - \rho_\mu| = 0. \tag{30}$$

The lower semicontinuity of entropy [3] gives

$$S(\bar\rho) \le \liminf S\big(\rho_\mu\big), \tag{31}$$

which together with the bound (25) establishes the convergence

$$\lim_{\mu\to 0} S(\rho_{\rm poly}) = S(\rho). \tag{32}$$

III. COUPLED HARMONIC OSCILLATORS

We illustrate our result by considering entanglement of the ground state of two oscillators with the Hamiltonian

$$H = \frac{1}{2m}(p_1^2+p_2^2) + \frac{m\omega^2}{2}(x_1^2+x_2^2) + \lambda(x_1-x_2)^2. \tag{33}$$

A parameter that determines the closeness of the physical prediction is the ratio of the lattice size μ to the oscillator scale

$$d = (m\omega)^{-1/2}. \tag{34}$$

The ground state of this Hamiltonian (in the Schrödinger quantization) is Gaussian [22, 23], i.e., all statistical moments of the canonical observables can be expressed from the first two moments — the expectation values and the variances. Ground states of any quadratic

n-particle Hamiltonian, as well as thermal states, coherent states and squeezed states are of this type. Gaussian states are very important in quantum optics and quantum information processing. They have a number of useful mathematical properties, of which we need two. First, a reduced density matrix of a Gaussian state (e.g., density operator of the first oscillator in the above example) is also Gaussian. Second, entropy of a Gaussian state can be calculated using its symplectic eigenvalues, as we now describe [7, 22].

Position and momenta (either classical or quantum) of n particles can be arranged into a single $2n$-dimensional vector $r^T = (x_1, \ldots, x_n, p_1, \ldots, p_n)$. Classical Poisson brackets and quantum commutation relations can be expressed using the $2n \times 2n$ symplectic matrix J,

$$\begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}, \qquad [r_k, r_k] = iJ_{kl}, \tag{35}$$

where I_n is the n-dimensional identity matrix, and the symplectic matrix satisfies $J^T = -J = J^{-1}$. The Hamilton equations are given by $\dot{r} = J\partial H/\partial r$, and the canonical transformations are represented by matrices S that satisfy $SJS^T = J$, thus forming the n-dimensional symplectic group.

The vector of expectation values and the symmetric correlation matrix are defined by

$$D = \langle \hat{r} \rangle, \qquad \Gamma_{ij} = \big\langle \{(\hat{r}_i - D_i), (\hat{r}_j - D_j)\} \big\rangle \tag{36}$$

where $\{a, b\}$ is the anticommutator. Unitary operators $U(S)$ that by transforming the Gaussian state according to $\rho' = U(S)\rho U^\dagger(S)$ transform the statistical moments according to

$$D' = SD, \qquad \Gamma' = S\Gamma S^T, \tag{37}$$

are called Gaussian operators. They represent important experimental procedures in quantum optics and quantum information.

Any Gaussian correlation matrix Γ can be diagonalized by some symplectic transformation S_W, $S_W \Gamma S_W^T = W$, where W is a diagonal matrix $\mathrm{diag}(\sigma_1, \ldots, \sigma_n, \sigma_1, \ldots, \sigma_n)$. This spectrum consists of the absolute values of the eigenvalues of the matrix $iJ\Gamma$. The eigenvalues σ_j are the symplectic eigenvalues of the covariance matrix. Finally, entropy of a n-particle Gaussian state ρ is given by its symplectic eigenvalues as [7, 23]

$$S(\rho) = \sum_{j=1}^{n} \left(\frac{\sigma_j + 1}{2} \log \frac{\sigma_j + 1}{2} - \frac{\sigma_j - 1}{2} \log \frac{\sigma_j - 1}{2} \right). \tag{38}$$

Covariance matrix of the ground state of a single harmonic oscillator (in the Schrödinger representation) is

$$\Gamma = \begin{pmatrix} 2\langle \hat{x}^2 \rangle & \langle \hat{x}\hat{p} \rangle + \langle \hat{p}\hat{x} \rangle \\ \langle \hat{p}\hat{x} \rangle + \langle \hat{x}\hat{p} \rangle & 2\langle \hat{p}^2 \rangle \end{pmatrix} = \begin{pmatrix} d^2 & 0 \\ 0 & d^{-2} \end{pmatrix}. \tag{39}$$

Calculations in the polymer representation also give zero expectations, $\langle \hat{x} \rangle = 0$, $\langle \hat{p}_\mu \rangle = 0$, but the variances are [11]

$$\langle \hat{x}^2 \rangle \approx \frac{d^2}{2} \left(1 - \frac{4\pi^2 d^2}{\mu^2} e^{-\pi^2 d^2/\mu^2} \right), \ \langle \hat{p}_\mu^2 \rangle \approx \frac{1}{2d^2} \left(1 - \frac{\mu^2}{2d^2} \right). \tag{40}$$

The correlation term vanishes exactly. Hence, keeping only the leading terms in μ/d the correlation matrix becomes

$$\Gamma_\mu = \begin{pmatrix} d^2 & 0 \\ 0 & \frac{1}{d^2}\left(1 - \frac{\mu^2}{2d^2}\right) \end{pmatrix} \tag{41}$$

The product of uncertainities the polymer quantisation is less than its standard value of $\frac{1}{4}$ [11, 24]. The state is no longer exactly Gaussian: because the correlation matrix violates the inequality $\Gamma_\mu + iJ \geq 0$, and Eq. (38) gives a complex value of the entropy, $S \sim i\frac{\mu^2}{d^2}$, for a pure state.

The standard measure of a pure state bipartite entanglement is the von Neumann entropy of either of the reduced density matrices [4]. For the Gaussian states it can be calculated using Eq. (38), whith symplectic eigenvalues for the correlation matrix of the subsystem. Tranforming to the normal modes (this is a simplectic transformation) gives two uncoupled oscillators with the frequencies

$$\omega_1 = \omega, \qquad \omega_2 = \omega_2 = \omega\sqrt{1 + \frac{4\lambda}{m\omega^2}} \equiv \omega\alpha. \tag{42}$$

The (Schrödinger) correlation matrix in the normal coordinates is $\Gamma' = \mathrm{diag}(d^2, d^2/\alpha, d^{-2}, d^{-2}\alpha)$, and the only eigenvalue of the reduced correlation matrix is

$$\sigma_1 = \frac{1 + \alpha}{2\sqrt{\alpha}}. \tag{43}$$

The polymer quantization is treated similarly. Assuming $\alpha > 1$ and keeping only the leading order terms in the powers of μ/d we find

$$\sigma_1^{\mathrm{poly}} = \sigma_1 - \frac{(1 + \alpha^2)}{8\sqrt{\alpha}} \frac{\mu^2}{d^2}, \tag{44}$$

and

$$S^{\mathrm{poly}} = S - \frac{1 + \alpha^2}{8\sqrt{\alpha}} \log \frac{\sqrt{\alpha} + 1}{\sqrt{\alpha} - 1} \frac{\mu^2}{d^2}. \tag{45}$$

IV. SUMMARY AND OUTLOOK

We showed that the shadow state construction gives not only "close" expectation values for the observables in the unitarily inequivalent representations, but the entropies of the two states agree as well. The lattice effects modify the expectation values and commutation relations. Shadow states do not satisfy the Gaussian property exactly, but only up to the terms of the order of μ^2/d^2.

Since the convergence of entropy of the shadow states to the Schrödinger representation value is not necessarily uniform, the following scenario is plausible. Both the discrepancy in the expectation of the momentum variances and symplectic eigenvalues are of the order of μ^2/d_j^2 for each (uncoupled) oscillator. This is also order of magnitude of the corresponding change in entropy contribution if Eq. (38) is used. Hence, even if the expectations of the observables agree, for a fixed value of μ and a large number n of oscillators the two entropies will differ by $\sim n\mu^2/d^2$, which may be a significant amount. We leave for future work a precise estimate of the discrepancy in entropies for a fixed scale and a large number of particles.

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